# FULLERENE ANIONS AND PAIRING IN FINITE SYSTEMS

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## INTRODUCTION

The discovery of superconductivity in alkali-metal-doped fullerenes[1] $K_3C_{60}$ and $Rb_3C_{60}$ has raised interesting questions about the electron-phonon coupling in such compounds and its interplay with Coulomb repulsion. $C_{60}$ is a highly symmetrical molecule i.e. it is a truncated icosahedron and its electronic lowest unoccupied molecular orbitals (LUMO) are threefold degenerate[2,3,4]. They form a $T_{1u}$ representation of the icosahedral group $\mathbf{I}_h$. Filling the LUMO in $C_{60}^{n-}$ anions leads in a naive picture to narrow, partially filled bands in the bulk fullerides. The bandwidth W is determined by the hopping between the $C_{60}$ molecules which are quite far apart and $W \approx 0.5$ eV. The coupling of some $H_g$ phonons with electrons residing in the $T_{1u}$ orbital has been suggested to be responsible for the superconductivity[5,6,7]. The Coulomb repulsion also may be important on the ball[8]. Several authors[9−12] have undertaken the study of the Jahn-Teller distortion that is expected in the fullerene anions. In such calculations one approach is to consider the electrons as fast degrees of freedom and the phonon normal coordinates are treated as static[13]. This is the strong-coupling approach to the Jahn-Teller effect. Of course it is more difficult to treat the fully dynamical problem of the phonon mode coupled to the electrons. Here we will investigate the interplay between the electronic and phononic degrees of freedom on an *isolated* fullerene anion. We use a *weak coupling* approach to the

Jahn-Teller effect The lifting of degeneracy is obtained by a perturbation calculation in the case of an undistorted anion. The ordering of levels can be described as "anti-Hund"' rule. This calculation is very close in spirit to the standard treatment of the electron-phonon coupling in superconducting metals. In fact we show that this weak-coupling approach is exactly parallel to the nuclear physics calculation of pairing of nucleons in a single shell. We recover the so-called seniority model of pairing. It is often claimed that "superconductivity is a dynamical Jahn-Teller effect". While such a statement is not very appropriate to bulk metallic superconductors, we will show that in the context of fullerene anions, it really makes sense. There is now some evidence that the crossover from weak to strong coupling in this Jahn-Teller problem is smooth[24], so the weak-coupling calculation captures the physics of the intermediate regime.

As in nuclear physics we find even-odd effects due to pairing in the ions. The effects we observe may be sought by spectroscopy of solutions of fullerides in liquid ammonia, for example. We discuss the opposite effect of Coulomb interaction, leading to Hund's rule in ordinary situations. Finally we point out that experimentally observed spectra may be at least partially explained by our calculation[23].

## THE ON-BALL ELECTRON-PHONON INTERACTION

The electronic structure of $\pi$ electrons in the $C_{60}$ molecule is well known to be given by a simple Hückel calculation. The levels are labeled[4] by the irreducible representations (irreps) of the icosahedron group $\mathbf{I_h}$. One important property has to be noted: three of the $\mathbf{I_h}$ irreps are the $l=0,1,2$ spherical harmonics of $\mathbf{SO(3)}$ which do not split under the $\mathbf{I_h}$ group. They are commonly named $A_g$, $T_{1u}$, $H_g$. In addition there is also the twofold spin degeneracy.

In the ground-state of the neutral $C_{60}$ molecule all levels up to $H_u$ included are completely filled thus building a singlet state $|\Psi_0\rangle$. The LUMO are the six $T_{1u}$ states. These are occupied upon doping with extra electrons and the ground-state becomes then degenerate. One then expects the Jahn-Teller effect to distort the anion and lift this orbital degeneracy[13,14]. due to the coupling of the $T_{1u}$ electrons to the vibrational modes of the molecule (also referred to as phonons). In a weak-coupling scheme the phonon is purely virtual and is exchanged between electrons. Phonon exchange between electrons leads to an effective electron-electron interaction that competes with Coulomb repulsion and may lead to anti-Hund ordering of energy-levels.

As a first investigation of electron-phonon coupling we use a perturbation scheme suited to degenerate levels we will derive an effective electron-electron interaction with the assumption that filled states lying below the $T_{1u}$ level remain frozen so that intermediate states involve only $T_{1u}$–$T_{1u}$ excitations. Indeed the $H_u$–$T_{1u}$ gap is $\approx 2eV$ whereas maximum phonon energies are $\approx 0.2eV$.

A typical electron-phonon interaction term reads:

$$W = \sum_{\alpha,m_1,m_2,\sigma} f_{\alpha m_1 m_2} X_\alpha c^\dagger_{m_1\sigma} c_{m_2\sigma}.$$

Here $X_\alpha$ are normal coordinates, the subscript referring both to the irrep and to the row in the irrep they belong to, $c^\dagger_{m_1\sigma}$ is the creation operator for an electron with spin $\sigma$ in the $T_{1u}$ ($l=1$) level, $m_1$ taking one of the $m=-1,0,1$ values, and $f_{\alpha m_1 m_2}$ are complex coefficients. The $c^\dagger_{m\sigma}$ operators transform as $l=1$ $|l, m\rangle$ vectors under $\mathbf{I_h}$ symmetries, and their conjugates $c_{m\sigma}$ transform as $(-1)^{m+1}|l, -m\rangle$ vectors. The $(-1)^{m_2+1}c^\dagger_{m_1\sigma}c_{-m_2\sigma}$ products transform then as members of the $T_{1u} \times T_{1u}$ representation, which in the $\mathbf{I_h}$ group splits as:

$$T_{1u} \times T_{1u} = A_g + T_{1g} + H_g.$$

This selects the possible vibrational modes $T_{1u}$ electrons can couple to. In fact, only $H_g$ modes split the degeneracy[7].

Let us consider a particular fivefold degenerate multiplet of $H_g$ modes. Their normal coordinates will be labelled $X_m$, $m$ ranging from -2 to +2. Since $H_g$ appears only once in the product $T_{1u} \times T_{1u}$, the interaction is determined up to one coupling constant $g$ by the usual formula for the coupling of two equal angular momenta to zero total angular momentum:

$$W = g\sum_m (-1)^m X_m \Phi_{-m}. \tag{1}$$

The $X_m$ may be chosen such that $X^\dagger_m = (-1)^m X_{-m}$ and have the following expression in terms of phonon operators:

$$X_m = \frac{1}{\sqrt{2}}\left(a_m + (-1)^m a^\dagger_{-m}\right) \tag{2}$$

whereas the $\Phi_m$ are the irreducible $l=2$ tensor operators built from the $c^\dagger c$ products according to:

$$\Phi_m = \sum_{m_1}(1, 1, 2|m_1, m - m_1, m)(-1)^{(m-m_1+1)}c^\dagger_{m_1\sigma}c_{-m+m_1\sigma}, \tag{3}$$

where $(l_1, l_2, l|m_1, m_2, m)$ are Clebsch-Gordan coefficients.

We now consider a doped $C_{60}^{n-}$, molecule, $0 \leq n \leq 6$. Its unperturbed degenerate ground-states consist of $|\Psi_0\rangle$ to which $n$ $T_{1u}$ electrons have been added times a zero-phonon state. They span a subspace denoted by $\mathcal{E}_0$. In $\mathcal{E}_0$ the unperturbed Hamiltonian $H_0$ reads:

$$H_0 = \epsilon_{t_{1u}}\sum_{m,\sigma}c^\dagger_{m\sigma}c_{m\sigma} + \hbar\omega\sum_m a^\dagger_m a_m,$$

where $\epsilon_{t_{1u}}$ is the energy of the $T_{1u}$ level, $\hbar\omega$ is the phonon energy of the $H_g$ multiplet under consideration. Within $\mathcal{E}_0$ the effective Hamiltonian up to second order perturbation theory is given by:

$$H_{eff} = E_0 P_0 + P_0 W P_0 + P_0 W(\mathbf{1} - P_0)\frac{1}{E_0 - H_0}(\mathbf{1} - P_0)W P_0,$$

3

where $P_0$ is the projector onto $\mathcal{E}_0$, $E_0$ is the unperturbed energy in this subspace which is just the number of doping electrons times $\epsilon_{t_{1u}}$. The linear term in $W$ gives no contribution. Using expressions (1) and (2) for $W$ and $X_m$ one finds:

$$H_{eff} = H_0 - \frac{g^2}{2\hbar\omega} \sum_{m,\sigma_1\sigma_2} (-1)^m \Phi_{m\sigma_1} \Phi_{-m\sigma_2}, \qquad (4)$$

where we have now included spin indices. We can now use equation (3) to express $H_{eff}$ as a function of $c$ and $c^\dagger$ operators and put it in normal ordered form using fermion anticommutation rules. In this process there appears a one-body interaction term which is a self-energy term. We will henceforth omit the $H_0$ term which is a constant at fixed number of doping electrons.

Let us now define pair creation operators $A_{lm}^{s\sigma\,\dagger}$ which when operating on the vacuum $|0\rangle$ create pair states of $T_{1u}$ electrons that are eigenfunctions of $\mathbf{L},\mathbf{S}$, $L_z,S_z$, where $\mathbf{L},\mathbf{S}$ are total angular momentum and spin, and $L_z,S_z$ their $z$-projections. $l$ and $s$ can take the values 0,1,2 and 0,1 respectively. This holds also if $|0\rangle$ is taken to be the singlet state $|\Psi_0\rangle$.

$$A_{lm}^{s\sigma\,\dagger} = \sum_{m_1,\sigma_1} (1,1,l|m_1, m-m_1, m)(\frac{1}{2},\frac{1}{2},s|\sigma_1,\sigma-\sigma_1,\sigma)c_{m_1\sigma_1}^\dagger c_{m-m_1\sigma-\sigma_1}^\dagger. \qquad (5)$$

The quantity $A_{lm}^{s\sigma\,\dagger}$ is non-zero only if $(l+s)$ is even and the norm of $A_{lm}^{s\sigma\,\dagger}|0\rangle$ is then equal to $\sqrt{2}$. The inverse formula expressing $c^\dagger c^\dagger$ products as $A^\dagger$ operators is:

$$c_{m_1\sigma_1}^\dagger c_{m_2\sigma_2}^\dagger = \sum_{l,s}(1,1,l|m_1,m_2,m_1+m_2)(\frac{1}{2},\frac{1}{2},s|\sigma_1,\sigma_2,\sigma_1+\sigma_2)A_{lm_1+m_2}^{s\sigma_1+\sigma_2\,\dagger}. \qquad (6)$$

As $H_{eff}$ is a scalar, its two-body part may be written as a linear combination of diagonal $A_{lm}^{s\sigma\,\dagger}A_{lm}^{s\sigma}$ products whose coefficients depend only on $l$ and $s$:

$$\sum_{ls,m\sigma} F(l,s)A_{lm}^{s\sigma\,\dagger}A_{lm}^{s\sigma}.$$

The $F(l,s)$ coefficients are calculated using expressions (4), (3), (6). We then get $H_{eff}$ in final form:

$$H_{eff} = -\frac{5g^2}{6\hbar\omega}\left(\hat{N} + A_{00}^{00\dagger}A_{00}^{00} - \frac{1}{2}\sum_{m,\sigma} A_{1m}^{1\sigma\,\dagger}A_{1m}^{1\sigma} + \frac{1}{10}\sum_{m} A_{2m}^{00\,\dagger}A_{2m}^{00}\right). \qquad (7)$$

In this formula $\hat{N}$ is the electron number operator for the $T_{1u}$ level; the $\hat{N}$ term appears when bringing $H_{eff}$ of expression (4) in normal ordered form. In our Hamiltonian formulation the effective interaction is instantaneous.

There are actually eight $H_g$ multiplets in the vibrational spectrum of the $C_{60}$ molecule. To take all of them into account we only have to add up their respective coefficients $5g^2/6\hbar\omega$, their sum will be called $\Delta$.

## THE ELECTRONIC STATES OF FULLERENE ANIONS

We shall now, for each value of $n$ between 1 and 6, find the $n$-particle states and diagonalize $H_{eff}$. The Hamiltonian to be diagonalized is that of equation (7) where the prefactor is replaced by $-\Delta$. The invariance group of $H_{eff}$ is $\mathbf{I_h} \times \mathbf{SU(2)}$. The $n$-particle states may be chosen to be eigenstates of $\mathbf{L}, \mathbf{S}, L_z, S_z$ and we shall label the multiplets by $(l, s)$ couples, in standard spectroscopic notation ($^{2s+1}$L stands for (l,s)). The pair $(l, s)$ label $\mathbf{SO(3)} \times \mathbf{SU(2)}$ irreps which, as previously mentioned, remain irreducible under $\mathbf{I_h} \times \mathbf{SU(2)}$ as long as $l$ doesn't exceed 2; for larger values of $l$ $\mathbf{SO(3)}$ irreps split under $\mathbf{I_h}$. Fortunately enough, the relevant values of $l$ never exceed 2. Moreover given any value of $n$, $(l, s)$ multiplets appear at most once so that the energies are straightforwardly found by taking the expectation value of the Hamiltonian in one of the multiplet states. The degeneracies of the levels will then be $(2l + 1)(2s + 1)$. We now proceed to the construction of the states.

- **n=1:** There are six degenerate $^2$P states $c_{m\sigma}^\dagger |\Psi_0\rangle$ whose energy is $-\Delta$.

- **n=2:** There are 15 states, generated by applying $A_{lm}^{s\sigma\,\dagger}$ operators on $|\Psi_0\rangle$. There is one $^1$S state, five $^1$D states and nine $^3$P states with energies $-4\Delta$, $-11\Delta/5$, $-\Delta$.

- **n=3:** There are 20 states. States of given $l, m, s, \sigma$ can be built by taking linear combinations of $A^\dagger c^\dagger |\Psi_0\rangle$ states according to:

$$\sum_{m_1,\sigma_1} (l_1, 1, l|m_1, m - m_1, m)(s_1, \frac{1}{2}, s|\sigma_1, \sigma - \sigma_1, \sigma) A_{l_1 m_1}^{s_1 \sigma_1\,\dagger} c_{m-m_1\sigma-\sigma_1}^\dagger |\Psi_0\rangle.$$

These states belong to the following multiplets: $^2$P (E=$-3\Delta$), $^2$D (E= $-9\Delta/5$), $^4$S (E=0).

- **n=4:** There are 15 states, which are obtained by applying $A_{lm}^{s\sigma\,\dagger}$ operators on $A_{00}^{00\,\dagger}|\Psi_0\rangle$. They are $^1$S (E=$-4\Delta$), $^1$D (E= $-11\Delta/15$), $^3$P (E=$-\Delta$)

- **n=5:** There are six $^2$P states which are $c_{m\sigma}^\dagger A_{00}^{00\,\dagger} A_{00}^{00\,\dagger}|\Psi_0\rangle$ and whose energy is $-\Delta$.

- **n=6:** There is one $^1$S state whose energy is 0.

It is interesting to note that the above treatment of electron-phonon interaction parallels that of pairing forces in atomic nuclei[15,16]. Of course in the case of finite fermionic systems there is no breakdown of electron number but there are well-known "odd-even" effects that appear in the spectrum. In our case pairing shows up in the $^1$S ground state for $C_{60}^{2-}$ rather than $^3$P as would be preferred by Coulomb repulsion i.e. Hund's rule. The construction of the states above is that of the seniority scheme in nuclear physics[16]. We note that similar ideas have been put forward by V. Kresin some time ago, also in a molecular context[17]. The effective interaction that he considered was induced by $\sigma$ core polarization.

## THE EFFECT OF COULOMB REPULSION

We now consider the Coulomb electron–electron interaction and assume it to be small enough so that it may be treated in perturbation theory. To get some feeling of the order of magnitude of this repulsion we use the limiting case of on-site interaction i.e. the Hubbard model. This Hamiltonian is not specially realistic but should contain some of the Hund's rule physics. The two-body interaction now reads:

$$\frac{U}{2} \sum_{i,\sigma} c_{i\sigma}^\dagger c_{i-\sigma}^\dagger c_{i-\sigma} c_{i\sigma},$$

where the $i$ subscript now labels the $\pi$ orbitals on the $C_{60}$ molecule. The quantity U is $\approx$ 2-3 eV from quantum chemistry calculations[18] Since level degeneracies are split at first order in perturbation theory we confine our calculation to this order and have thus to diagonalize the perturbation within the same subspace $\mathcal{E}_0$ as before. In this subspace it reads:

$$W_H = U \sum_{i,\alpha\beta\gamma\delta} \langle\alpha|i\rangle\langle\beta|i\rangle\langle i|\gamma\rangle\langle i|\delta\rangle \; c_{\alpha\uparrow}^\dagger c_{\beta\downarrow}^\dagger c_{\gamma\downarrow} c_{\delta\uparrow},$$

where greek indices label one–particle states belonging either to $|\Psi_0\rangle$ or to the $T_{1u}$ level. Let us review the different parts of $W_H$. Note that since the $|\Psi_0\rangle$ singlet remains frozen we have the identity: $c_\alpha^\dagger c_\beta = \delta_{\alpha\beta}$ if $\alpha,\beta$ label states belonging to $|\Psi_0\rangle$.

–A part involving states belonging to $|\Psi_0\rangle$ only:

$$W_{H_1} = U \sum_{i,\alpha\beta} |\langle\alpha|i\rangle|^2 |\langle\beta|i\rangle|^2 \; c_{\alpha\uparrow}^\dagger c_{\alpha\uparrow} \; c_{\beta\downarrow}^\dagger c_{\beta\downarrow}.$$

$\alpha,\beta$ belong to $|\Psi_0\rangle$. This term is thus diagonal within $\mathcal{E}_0$ and merely shifts the total energy by a constant that does not depend on the number of doping electrons. It won't be considered in the following.

–A part involving both states belonging to $|\Psi_0\rangle$ and to the $T_{1u}$ level:

$$W_{H_2} = U \sum_{i,\alpha\delta,\beta,\sigma} \langle\alpha|i\rangle\langle i|\delta\rangle |\langle\beta i|\rangle|^2 \; c_{\alpha\sigma}^\dagger c_{\delta\sigma} \; c_{\beta-\sigma}^\dagger c_{\beta-\sigma},$$

where $\alpha,\delta$ belong to the $T_{1u}$ level whereas $\beta$ belongs to $|\Psi_0\rangle$. It reduces to:

$$W_{H_2} = U \sum_{\alpha\delta,\sigma} c_{\alpha\sigma}^\dagger c_{\delta\sigma} \left( \sum_i \langle\alpha|i\rangle\langle i|\delta\rangle \sum_\beta |\langle\beta|i\rangle|^2. \right)$$

The sum over $\beta$ is just the density on site i for a given spin direction of all states belonging to $|\Psi_0\rangle$ which is built out of completely filled irreps. As a result this

density is uniform and since $|\Psi_0\rangle$ contains 30 electrons for each spin direction it is equal to $1/2$. $W_{H_2}$ then becomes diagonal and reads:

$$W_{H_2} = \frac{U}{2} \sum_{\alpha,\sigma} c^\dagger_{\alpha\sigma} c_{\alpha\sigma}.$$

Its contribution is thus proportional to the number of $T_{1u}$ electrons. It represents the interaction of the latter with those of the singlet and we won't consider it in the following.

–A part involving only states belonging to the $T_{1u}$ level:
$W_{H_3}$ has the same form as $W_H$ with all indices now belonging to the $T_{1u}$ level. Whereas the interaction has a simple expression in the basis of $|i\rangle$ states, we need its matrix elements in the basis of the $T_{1u}$ states. There are in fact two $T_{1u}$ triplets in the one–particle spectrum of the $C_{60}$ molecule, the one under consideration having higher energy. To construct the latter we have first constructed two independent sets of states which transform as $x, y, z$ under $\mathbf{I_h}$. These are given by:

$$|\alpha\rangle = \sum_i \vec{e}_\alpha . \vec{r}_i \, |i\rangle \quad \text{and} \quad |\alpha\rangle' = \sum_i \vec{e}_\alpha . \vec{k}_i \, |i\rangle,$$

where $\vec{e}_\alpha$ are three orthonormal vectors, $i$ labels sites on the molecule, the $\vec{r}_i$ are the vectors joining the center of the molecule to the sites while the $\vec{k}_i$ join the centre of the pentagonal face of the molecule the site $i$ belongs to to the site i. We assume that the bonds all have the same length. These states span the space of the two $T_{1u}$ triplets. The diagonalization of the tight–binding Hamiltonian in the subspace of these six vectors yields then the right linear combination of the $|\alpha\rangle$ and $|\alpha\rangle'$ states for the upper lying triplet. From the $x, y, z$ states one constructs $l=1$ spherical harmonics. We then get the matrix elements of $W_{H_3}$ in the basis of $T_{1u}$ states. As $\mathcal{E}_0$ is invariant under $\mathbf{I_h}$ operations and spin rotations, $W_{H_3}$ which is the restriction of $W_H$ to $\mathcal{E}_0$ is invariant too. It may thus be expressed using the $A$, $A^\dagger$ operators by using formula (5) in the same way as the phonon–driven interaction and we finally get:

$$W_{H_3} = \left( \frac{U}{40} A^{00\dagger}_{00} A^{00}_{00} + \frac{U}{100} \sum_m A^{00\ \dagger}_{2m} A^{00}_{2m} \right), \tag{8}$$

which is the only part in $W_H$ that we will keep. Note that there is no contribution from $l=1$, $s=1$ $A^\dagger A$ products. Indeed the Hubbard interaction is invariant under spin rotation and couples electrons having zero total $S_z$. As the coefficients of $A^\dagger A$ products depend solely on $l$ and $s$ they must be zero for $s \neq 0$. The spectrum for any number of $T_{1u}$ electrons is now easily found. Of course the order of the multiplet is now reversed: for n=2, we have $^3$P, then $^1$D, then$^1$S. For n=3, we have $^4$S, then $^2$D, then $^2$P. For n=4, we have $^3$P, then $^1$D, then $^1$S.

## CONCLUSION

The ordering of energy levels in the electron-phonon scheme are clearly opposite to those of Hund's rule. The clear signature of what we can call "on-ball" pairing is the ground state $^1$S of $C_{60}^{2-}$: the two extra electrons are paired by the electron-phonon coupling. We note that the U of the Hubbard model appears divided by large factors: this is simply due to the fact that the $C_{60}$ molecule is large. As a consequence, if U $\approx$ 2 eV, Coulomb repulsion may be overwhelmed by phonon exchange. With a $H_g$ phonon of typical energy 100 meV and coupling O(1) as suggested by numerous calculations[6,7,10], the quantity $\Delta$ may be tens of meV.

It seems to us that the cleanest way to probe this intramolecular pairing would be to look at solutions of fullerides leading to free anions such as liquid ammonia solutions or organic solvents[19−22]. EPR or IR spectroscopy should be able to discriminate between the two types of spectra. Measurements by EPR should determine whether or not the two extra electrons in $C_{60}^{2-}$ are paired, for example. In near-IR spectroscopy the lowest allowed transition for $C_{60}^{2-}$ should be at higher energy than that of $C_{60}^{-}$ due to the pairing energy while in the Coulomb-Hubbard case it is at lower energy.

Present experiments[19,20] have studied the near-IR spectra of solutions of fulleride anions prepared by electrochemical reduction. There are several peaks that do not fit a simple Hückel scheme of levels. They do not have an immediate interpretation in terms of vibrational structure[19,20]. With our energy levels in table I, a tentative fit would lead to $\Delta \approx 80$ meV assuming U = 0. Such a value leads to intriguing agreement with the major peaks seen for $C_{60}^{2-}$ and $C_{60}^{3-}$ while this is no longer the case for $C_{60}^{4-}$ and $C_{60}^{5-}$.

Finally we mention that recent EPR experiments[22] have given some evidence for non-Hund behaviour of the fulleride anions. While one may observe some trends similar to the results of the phonon-exchange approximation, it is clear that the model we used is very crude. In a bulk *conducting* solid we do not expect the previous scheme to be valid since the levels are broadened into bands: then phonon exchange leads of course to *superconductivity*.

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